Implementation of Strain Induced Effects in Sensor Device Simulation

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ABSTRACT

Device simulation technique is applied to the piezoresistive sensor by including the doping profile and the strain distribution in the silicon substrate. In this simulation, the device equations are solved by Newton's method taking into account the anisotropic mobilities of carriers induced by strain, which results in affecting the change of the carriers concentrations at each node. Simulation is done through an algorithm developed in 'SGFramework'. Modeling of the implementation of strain induced effects in the device simulation is shown and its feasibility is discussed.

Keywords: sensor, device simulation, PDE, piezeresistance, stress, impurity.

INTRODUCTION

Device simulation is the technique that have been developed to design the VLSI and specify the current behavior in semiconductors, which will be applied to the solid state sensors if the implementation of sensing part can be performed.

There are many kinds of stress calculations on various diaphragm configuration of the piezoresistive (PR) sensor [1], [2], but very few on the current behavior. Previously we simulated the influence of heavy doping for the temperature coefficient of PR sensor [3], in which the impurity band and the tail of the band edge formed by the interaction of the impurity atoms were treated as the density of states functions, and then "effective band-gap narrowing" was figured out.

However proper modeling for the current behavior in sensor device simulation have not been realized yet. In the present study we explored the PR sensor simulation by implementing the strain induced effects and the doping profile of silicon in the device simulation.

Two methods are widely used in the device simulation: the method to solve the valance equations and the Monte-Carlo (MC) method for the carrier transport processes. We adopt the former since it is more convenient simulation in getting along with the conventional FEM stress calculation.

In modeling the PR sensor the strain affects in two ways. Firstly it brings about additional variation in the concentration of carriers localized in the doped region. For example, the shrink of material , as well as heavily doping, makes the energy gap between the band edge and the quasi-Fermi level narrower, which makes the density of carriers in this shrunk region increase. Secondly, the mobilities of carriers are also changed by strain.

We investigate our sensor simulation through an algorithm developed in 'SGFramework' [4]. It provides highly flexible partial differential equations (PDEs) solver for numerical solution of large-scale computational problems in applied physics, and includes excellent tools needed to solve the device equations such as translator to C++ code, mesh generation program, refinement program, etc.

SENSOR SIMULATION SCHEME

The basic semiconductor device equations consist of three coupled PDEs: Poisson's equation, an electron continuity equation and a hole continuity equation. In order to solve these device equations the finite-difference method is popularly used [5]. In this procedure the simulation domain is divided into meshes and the values appeared in the PDEs are discretized at node which is the vertex of the meshes. By this discretization procedure, the Poisson's equation becomes the box integration and the continuity equations become the central-difference approximation or the Scharfetter-Gummel discretization [7].

Then discretizing a system of PDEs on an appropriate solution mesh results in a system of algebraic equations which are coupled and usually nonlinear. These algebraic equations are solved via Newton's method for nonlinear system. At each iteration of Newton's method, the linear system is solved via, say, Gauss-elimination algorithm.

As for our overview of the sensor simulation, we should conmbine our model presented in this study with other CAD tools for MEMS which will provide the process and mechanical data of the diaphragm fabricated as the piezoresistive sensor device (Fig.1).

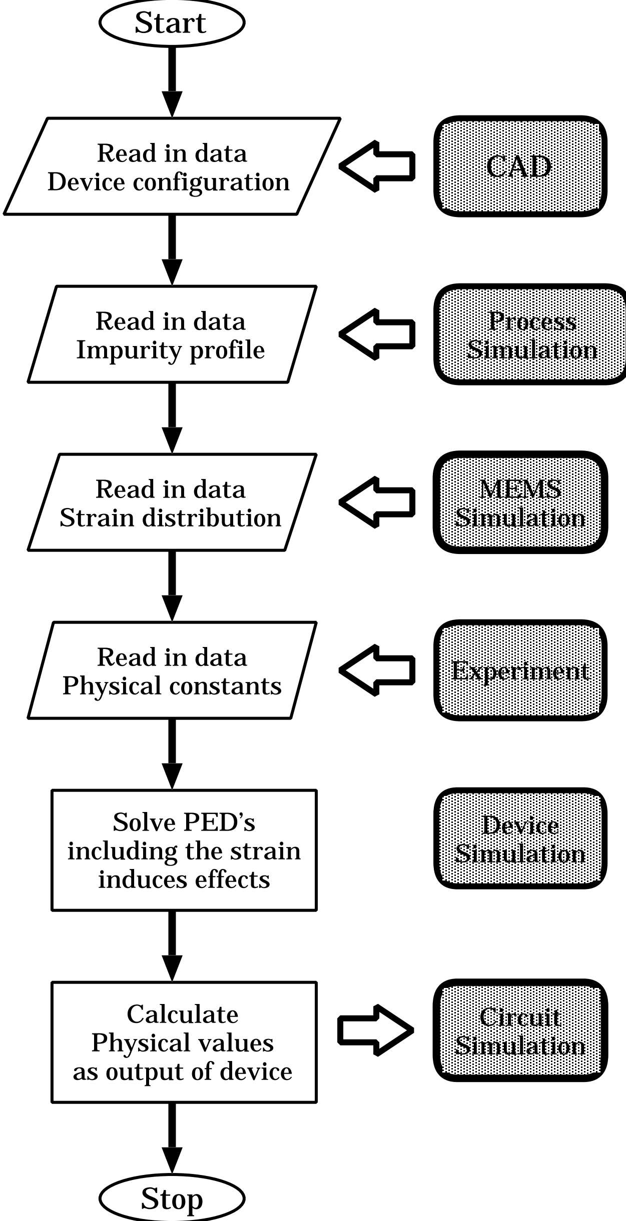

Figure 1: Flow chart of sensor device simulation

Stress Induced Effects

When mechanical stress is applied to a semiconductor substrate, a strain is induced in the crystal which affects its resistivity, that is the PR effect. The purpose of the present paper is to attempt to implement this PR effect in the aforementioned device simulation. Before getting onto the implementation, we briefly review the expression of the PR effect in silicon [8].

PR effects can be expressed as the change of conductivity induced by stress:

$$\sigma_{lm} = \sigma_0(\delta_{lm} - \sum_{i,j} \pi_{lmij} P_{ij}), \tag{1}$$

where σ_{lm} is the conductivity component, P_{ij} is the stress component, π_{lmij} is the PR coefficient component. In an unstressed crystal, σ_{lm}'s are independent of subscripts and σ_{ll}'s equal to σ_0 and $\sigma_{lm}(l \neq m)$'s vanish. Because of the crystallographic nature, the stress in the material is described by a second rank tensor and PR coefficients are described by a forth tank tensor. The symmetry of diamond structure reduces the numbers of independent components of π_{lmij}'s to three.

In general, the conductivity is a second rank tensor, which is expressed as (2) and defined by the current components J_l's and the electric field components E_m's.

$$J_l = \sum_m \sigma_{lm} E_m. \tag{2}$$

In a strained silicon, the conductivity dose not only changes its magnitude, but also becomes to have an anisotropic property, whose tensor has off-diagonal components.

The above expressions are defined with reference to the principal crystal axes. They usually required in an arbitrary oriented coordinate system. In order to calculate them for arbitrary crystallographic directions, a tensor transformation of the coordinate system shall be applied. In this transformation, we consider a Cartesian system whose three axes have direction cosines $[l_1 m_1 n_1]$, $[l_2 m_2 n_2]$ and $[l_3 m_3 n_3]$ with respect to the principal crystal axes. We denote by prime tensor components in the new coordinate system. The transformations of current, electric field, conductivity, stress tensor and PR coefficient are expressed as follows,

$$J_l^{'} = \sum_k a_{lk} J_k, \qquad E_m^{'} = \sum_k a_{mk} E_k \tag{3}$$

$$\sigma_{pq}^{'} = \sum_{r,s} a_{pr} a_{qs} \sigma_{rs}, \quad P_{pq}^{'} = \sum_{i,j} a_{pi} a_{qj} P_{ij} \tag{4}$$

$$\pi_{pqkn}^{'} = \sum_{l,m,i,j} a_{pl} a_{qm} a_{ki} a_{ki} a_{nj} \pi_{lmij} \tag{5}$$

A typical coordinate system may be selected by making the new axis $3^{'}$ vertical to the plane of an (lmn) silicon wafer, that is,

$$[l_3 m_3 n_3] = (l^2 + m^2 + n^2)^{-1/2} [lmn], \tag{6}$$

and making the new axis $1'$ horizontal to the orientation flat of the wafer.

Implementation in Simulation

The discretized device equations of time-independent are given by (7), (8) and (9), which are corresponding to the Poisson's equation, the electron and hole continuity equations, respectively.

$$\lambda^2 \sum_j \left(\epsilon_r E \mid_{\mathrm{mid}(i,j)} L_j \right) = (p_i - n_i + C_i) A_i \quad (7)$$

$$+\sum_j \left(J^n \mid_{\mathrm{mid}(i,j)} L_{(i,j)} \right) - R_i A_i = 0 \quad (8)$$

$$-\sum_j \left(J^p \mid_{\mathrm{mid}(i,j)} L_{(i,j)} \right) - R_i A_i = 0 \quad (9)$$

where λ^2 is a small dimensionless scale factor, node i is an arbitrary interior node in the simulation domain, index j is the jth neighbor of node i, $E \mid_{\mathrm{mid}(i,j)}$ is the electric-field, R_i is the net recombination rate par unit volume, L_j is the length of the integration edge, A_i is the area of the integration box, $L_{(i,j)}$ is the length between the two jth neighbors of node i, n_i, p_i and C_i are the electron, hole and the net positive ionized ion concentrations, respectively. R_i is composed of Shockley-Read-Hall recombination, Auger recombination and avalanche generation, and is the function of n_i and p_i. The notation $u \mid_{\mathrm{mid}(i,j)}$ represents the quantity u at the midpoint of the edge which connects nodes i and j.

Then there are three unknown variables $E \mid_{\mathrm{mid}(i,j)}$, $J^n \mid_{\mathrm{mid}(i,j)}$ and $J^p \mid_{\mathrm{mid}(i,j)}$ in the above device equations, which should be substituted for V_i, n_i and p_i by using following equations: electric field (10), electron and hole continuity equations (11),(12). Since the latter variables are directly defined at each node, this substitution make a system of algebraic equations straightforward.

$$E \mid_{\mathrm{mid}(i,j)} = -(V_j - V_i)/h_{(i,j)}, \quad (10)$$

$$J^n \mid_{\mathrm{mid}(i,j)} = \mu^n_{(i,j)} \{ n \mid_{\mathrm{mid}(i,j)} E \mid_{\mathrm{mid}(i,j)} + D^n_{i,j} (n_j - n_i)/h_{i,j} \}, \quad (11)$$

$$J^p \mid_{\mathrm{mid}(i,j)} = \mu^p_{(i,j)} \{ p \mid_{\mathrm{mid}(i,j)} E \mid_{\mathrm{mid}(i,j)} + D^p_{(i,j)} (p_j - p_i)/h_{i,j} \}, \quad (12)$$

where V_i is the electrostatic potential at node i, $h_{(i,j)}$ is the length of the edge which connects nodes i and j, $\mu^{n,p}_{(i,j)}$ and $D^{n,p}_{(i,j)}$ are the carrier mobilities and the carrier diffusion coefficients from i to the jth node, respectively. The carrier mobilities and diffusion coefficients obey the Einstein relationship.

$$D^{n,p}_{(i,j)} = \frac{k_B T}{q} \mu^{n,p}_{(i,j)} \quad (13)$$

The carrier mobilities are influenced by several kinds of scattering mechanisms such as phonon scattering, ionized impurity scattering, neutral impurity scattering etc., and are the functions of temperature and impurity concentrations. In order to combine them, Dorkel and Leturcq approximation is available.

In the implementation of the strain induced effects in the device simulation, V_i, n_i and p_i should be treated as the functions of strain. However, there are some crucial problems to deal with the anisotropic property of the conductivity.

DISCUSSIONS

We would like to consider how the implementation of the PR effects in the device equations is achieved. The theory of the PR effect for n-type semiconductors was given by Herring & Vogt [9], and that for p-type was given by Pikus & Bir [10], which are summarized as follows. A strain in a crystal induces a shift of the band extrema which causes carrier transfer between these valleys, and also induces an effective mass shift for p-type semiconductors. Both of them cause an anisotropic nature in the conductivity.

There seems to be two ways to implement the PR effects, that is to make the carriers concentrations or the carriers mobilities have the stress dependency. By the way, the pn-product (14) is usually adopted in the device simulation to evaluate the band-gap narrowing by the temperature and the dopant concentrations.

$$pn = n_{ie}^2(N,T) = n_{i0}^2(T) \exp\left(\frac{q}{k_B T} \Delta V_{g0}(N) \right), \quad (14)$$

where ΔV_{g0} is the effective band-gap narrowing, N is the net doping concentration.

From the view point of the theory of the band extrema shift, it looks like plausible that the stress dependency of the carrier concentrations can be implemented by modifying the pn-product, however, this implementation becomes more complex because we must make the carrier concentrations have an anisotropic property. Keyes figured out that the strain in crystal degenerates the band edge energies and causes a change of the scattering rate between the non-equivalent valleys, and Hälg and our previous experimental results also supported to his theory [11]. Then we try to implement the stress dependency in the carriers mobilities.

Finally, we come to discuss the implementation of the anisotropic mobility. There are two difficult points to accomplish this procedure. Firstly, the treatment of the tensor values makes the solution of device equations difficult. The strain tensor affects several values in the device equations and three dimensional expressions. In a strained crystal the carrier mobilities become a second rank tensor, whose components are calculated from the definition of the PR coefficients and expressed as (17).

Then we can calculate the current vector components which are expressed as (16) and defined by the electric field vector components (15) and the obtained mobility tensor components,

$$E_u = -(V_j - V_i)/(u_j - u_i) \quad (u = x, y, z), \qquad (15)$$

$$J_v = \sum_u \mu_{vu} n \mid_{\mathrm{mid}(i,j)} E_u \mid_{\mathrm{mid}(i,j)} \quad (v = x, y, z), \qquad (16)$$

$$\mu_{lm} = \mu_{lm} \mid_{\mathrm{mid}(i,j)} \left(\delta_{lm} - \sum_{u,v} \pi_{lmuv} P_{uv} \mid_{\mathrm{mid}(i,j)} \right) \quad (l, m, u, v = x, y, z), \qquad (17)$$

where J_v and μ_{lm} are defined by both n- and p-type materials. The magnitude and the turn of the current flow from the i node to the jth neighbor are defined by $J = sign(E \mid_{\mathrm{mid}(i,j)})(J_x^2 + J_y^2 + J_z^2)^{1/2}$. Above equations should be replaced by (10), (11) and (12). Secondly, we must select a coordinate system in order to define the tensors components. However, we can adopt the aforementioned coordinate system.

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